An Adiabatic Theorem without a Gap Condition

J. E. Avron and A. Elgart
Department of Physics, Technion, 32000 Haifa, Israel

February 7, 2008

Abstract

The basic adiabatic theorems of classical and quantum mechanics are overviewed and an adiabatic theorem in quantum mechanics without a gap condition is described.

1 Classical Adiabatic Invariants

Consider a (mathematical) pendulum whose period is slowly modulated, for example by shortening the length of the pendulum, fig 1, [1, 18].

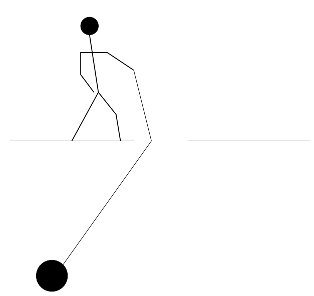

Figure 1: An adiabatic pendulum

The Hamiltonian describing the system is

$$H(s) = \frac{1}{2}\left(p^2 + \omega^2(s)\, x^2\right), \quad s = \frac{t}{\tau}. \tag{1}$$

t is the physical time, τ is the time scale. The adiabatic limit is $\omega\tau >> 1$. The period $\omega(s)$ is a smooth function which is time independent in the past, $s < 0$, and in the distant future, $s > 1$. A graph showing a possible variation of $\omega(s)$ is shown in fig. 2.

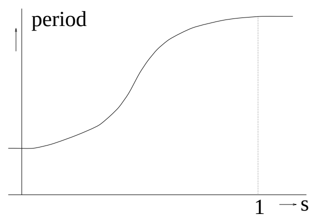

Figure 2: An adiabatic variation

An adiabatic invariant is an approximately conserved quantity whose deviation from constant can be made arbitrarily small for large τ, uniformly in s and *for all times*. For the Harmonic oscillator the adiabatic invariant is

$$S(s)=\frac{H(s)}{\omega(s)}. \tag{2}$$

The special properties of this particular combination of H and ω can be seen from its equations of motion:

$$\dot S(s)=\frac{\dot\omega(s)}{2\,\omega^2(s)}\,\left(\omega^2(s)\,x^2-p^2\right). \tag{3}$$

$\dot S$ is compactly supported (because $\dot\omega$ is), and appears to be $O(1)$ in τ. But, for the (time independent) Harmonic oscillator the time average over one period of the kinetic energy equals the time average of the potential energy. So, for large τ, the change of S in one period is small: $\langle\Delta S\rangle=O\left(\frac{1}{\tau}\right)$. Because of this adiabatic invariants give precise information on the long time behavior even though the total variation in the Hamiltonian is finite.

A remarkable fact about adiabatic invariants is that *for large times* the error is essentially exponentially small with τ if $\omega(s)$ is smooth [18]:

$$|S(s)-S(0)|=O\left(\frac{1}{\tau^\infty}\right),\quad s>1. \tag{4}$$

(The error is, in general, not exponentially small for $0<s<1$.) In certain circles an exponentially small error is sometimes taken to be the defining property of adiabatic invariant, so that proving an adiabatic theorem it taken to imply proving an exponentially small bound on the error. This, to our opinion, is not a satisfactory definition of the notion of adiabatic invariant, and instead we shall stick with the definition given above, namely, that adiabatic invariants are conserved up to an error that is uniformly bounded for all times, and can be made arbitrarily small with τ.

A link of classical adiabatic invariants with quantum mechanics that was emphasized by Ehrenfest [10] focused on the observation that adiabatic invariants

are related to quantum numbers. For the (time independent) Harmonic oscillator the particular combination of H and ω in Eq. (2) is a function of quantum numbers:

$$\frac{E}{\omega} = \hbar\left(n + \frac{1}{2}\right). \tag{5}$$

2 The Quantum Adiabatic Theorem

Ehrenfest observation had much influence in the early days of quantum mechanics, and in particular motivated the work of Born and Fock [8] on the adiabatic theorem of quantum mechanics. In quantum theory one is interested is solving the initial value problem

$$i\,\partial_t\psi = H(s)\,\psi, \quad s = \frac{t}{\tau}, \tag{6}$$

with ψ a vector in Hilbert space and $H\left(\frac{t}{\tau}\right)$ a self adjoint operator. We shall assume, as we did in the previous section, that $H(s)$ is time independent in the past, $s < 0$, and distant future, $s > 1$, and is a smooth operator valued function of s. In the case that $H(s)$ is an unbounded operator, like the Schrödinger operator, the notion of smoothness needs some clarification. We shall not get into this here.

Changing variables one writes the initial value problem as

$$i\,\dot{\psi} = \tau\,H(s)\,\psi. \tag{7}$$

The adiabatic limit is $\tau \to \infty$. Adiabatic theorems in quantum mechanics relate the solutions of the initial value problem to spectral properties.

The oldest result of this kind is due to Born and Fock who studied Hamiltonians with *discrete and simple* spectrum, fig. 3.

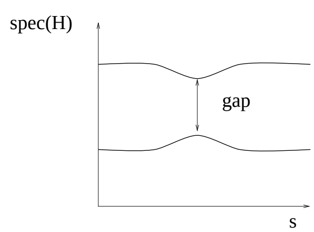

Figure 3: Spectrum in Born Fock Theory

Born and Fock showed that if the initial data are $\psi(0) = \phi(0)$, with $\phi(0)$ an eigenvector of $H(0)$, then $\psi(s)$ is close to an eigenvector $\phi(s)$ of $H(s)$ with particular choice of phase:

$$\|\psi(s) - \phi(s)\| = O\left(\frac{1}{\tau}\right). \tag{8}$$

For large times, $s > 1$, outside the support of $\dot{H}(s)$, much stronger result hold: the error is essentially exponentially small in τ, see e.g. [6, 15, 17, 21].

3 The Adiabatic Theorem of Kato

Kato generalized the result of Born and Fock. He showed that the assumption of spectral simplicity of $H(s)$ can be removed, and so can the assumption that the spectrum is discrete, fig. 4. These generalizations are important for applications to atomic physics where some continuous spectrum is always present, and degeneracies are ubiquitous. But, perhaps more importantly, Kato introduced an essentially new method of proving the adiabatic theorem that we shall now describe.

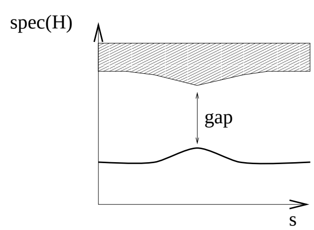

Figure 4: Spectrum in Kato's Theory

Kato's idea was to introduce a geometric evolution which satisfies the adiabatic theorem without an error. That is, a unitary $U_a(s)$, so that:

$$U_a(s)\,P(0) = P(s)\,U_a(s), \tag{9}$$

where $P(s)$ is a spectral projection for $H(s)$, and $U_a(0) = 1$. The second step is to compare the physical evolution, $U(s)$, generated by

$$i\,\dot{U}(s) = \tau\,H(s)\,U(s), \quad U(0) = 1. \tag{10}$$

with U_a and show that the two are close.

It turns out that both steps involve looking into commutator equations. If we let $H_a(s)$ denote the generator of the geometric evolution $U_a(s)$, it is not difficult to see that it must satisfy

$$\tau\,[H_a(s), P(s)] = i\,\dot{P}(s). \tag{11}$$

Using the fact that for any projection P

$$P(s)\,\dot{P}(s)\,P(s) = 0, \tag{12}$$

one checks that

$$H_a(s) = H(s) + \frac{i}{\tau}\,[\dot{P}(s), P(s)], \tag{13}$$

solves the commutator equation, with $H_a(s)$ which is manifestly close to $H(s)$.

To compare $U(s)$ and $U_a(s)$ let $\Omega(s) = U_a^*(s)\,U(s)$, $\Omega(0) = 1$. Using the equation of motion one finds

$$\dot{\Omega}(s) = i\,\tau\,U_a^*(s)\,(H_a(s) - H(s))\;U(s) = -U_a^*(s)[\dot{P}(s), P(s)]\,U(s), \tag{14}$$

which is compactly supported (since $\dot{P}(s)$ is) and $O(1)$ in τ. Now, like the situation for the classical adiabatic invariants, even though $\dot{\Omega}$ is not small, the change in Ω is small. This is where a second commutator equation enters. Suppose that the commutator equation

$$[H(s), X(s)] = [\dot{P}(s), P(s)] \tag{15}$$

has a smooth and bounded solution $X(s)$. Then,

$$\begin{aligned}
-\,\dot{\Omega}(s) &= U_a^*(s)[H(s), X(s)]\,U(s) = \\
&= U_a^*(s)\,(H_a(s)\,X(s) - X(s)\,H(s))\;U(s) + O\left(\frac{1}{\tau}\right) \\
&= \frac{i}{\tau}\left(\dot{U}_a^*(s)\,X(s)\,U(s) + U_a^*(s)\,X(s)\,\dot{U}(s)\right) + O\left(\frac{1}{\tau}\right) \\
&= \frac{i}{\tau}\left(\overset{\cdot}{\left(U_a^*(s)\,X(s)\,U(s)\right)} - U_a^*(s)\,\dot{X}(s)\,U(s)\right) + O\left(\frac{1}{\tau}\right).
\end{aligned} \tag{16}$$

From this it follows that $\Omega(s) - 1 = O\left(\frac{1}{\tau}\right)$.

The gap condition is a condition for the solvability of the commutator equation, Eq. (15). Indeed, suppose there is a gap in the spectrum so that the spectral projection P is associated with a contour Γ in the complex plane that lies entirely in the resolvent set, Fig. 5.

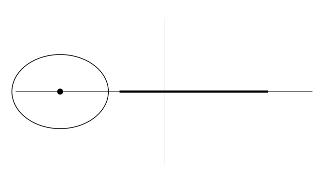

Figure 5: A contour Γ in the Complex Plane

A solution to the commutator equation is

$$X(s) = \frac{1}{2\pi i}\int_\Gamma R(s,z)\,\dot{P}(s)\,R(s,z)\,dz. \tag{17}$$

And, as usual $R(s,z) = (H(s) - z)^{-1}$ is bounded for $z \in \Gamma$. If the size of the gap is g then

$$\|X(s)\| = O\left(\frac{1}{g}\right). \tag{18}$$

Using Kato's method various adiabatic theorems have been proven see e.g. [3, 4, 17, 21].

4 The Role of the Gap Condition

The adiabatic theorem described in the previous section relied on a gap condition. How serious is this?

In the proof of Kato the gap condition guarantees the existence of a bounded solution to the commutator equation given by $X(s)$ of Eq. (17). The bound Eq.(18) blows up at the gap shrinks to zero and there is no *a-priori* bounded solution to the commutator equation. This suggests that the gap condition is essential.

A second argument leading to the same conclusion is a dimensional argument. The adiabatic limit needs a intrinsic time scale so that τ can be measured in dimensionless units. Otherwise the notion of large τ depends on a choice of a unit and is meaningless. In the case of the classical Harmonic oscillator the intrinsic time scale is set by ω. In the quantum case, a gap and Planck constant dictates an intrinsic time scale. In the absence of a gap, this time scale is lost. This suggests that the gap condition is essential and there should be no *general* adiabatic theorem in its absence.

Let us now describe two arguments that say the opposite. The first refers once again to the work of Born and Fock. Born and Fock (and also Kato) considered the more delicate adiabatic theorem for crossing energy levels, Fig. 6, and proved an adiabatic theorem in this case

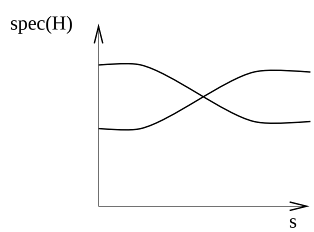

Figure 6: Crossing Eigenvalues in Born Fock Theory

Since the energy levels cross, the gap closes. For the case of linear crossing Born and Fock showed that Eq. (8) is replaced by

$$\|\psi(s) - \phi(s)\| = O\left(\frac{1}{\sqrt{\tau}}\right). \tag{19}$$

The time scale for this problem is dictated by the slope of the energy curves at the crossing point. These results have since been considerably strengthened and extended [12]. This suggests that a gap conditions controls the rate at which the adiabatic limit is approached, but an adiabatic theorem does not really require a gap condition.

A second argument supporting the view that a gap condition is only technical is a physical argument. Gaps in the spectrum are indeed prevalent in quantum mechanical systems, but they are no gaps in quantum electrodynamics: The interaction with radiation eliminates the gaps. Suppose that a charged quantum mechanical system, initially at the ground state, is slowly rotated. The adiabatic theorem would fail if the number of photons generated by the slow rotation does not go to zero in the adiabatic limit. Let us estimate this number [1]. The power radiated by a charged system in classical electrodynamics is proportional to the acceleration squared, i.e. to τ^{-4}. Hence the total radiated energy is of the order τ^{-3}. Since a typical radiated photon will, presumably, have frequency of order $\frac{1}{\tau}$ the number of radiated photons is of order τ^{-2}. This goes to zero in the adiabatic limit. This argument, in spite of its shortcomings, suggests that the gap condition, at least in the context of QED, is not really essential.

5 Removing the Gap Condition

A general adiabatic theorem without a gap condition was given in [2]. The point is that all the adiabatic theorem really needs is a distinguished smooth family of finite dimensional spectral projections, so that the adiabatic evolution has a distinguished subspace to follow. The proof works for eigenvalues embedded in some essential spectrum, or for eigenvalues at the threshold of essential spectrum, as one would expect to find in QED, fig. 7. It is essential for this result that the distinguished spectral subspace is *finite dimensional*. Let us begin by stating the theorem:

Theorem: Suppose that $P(s)$ is a finite rank spectral projection, which is at least twice differentiable (as a bounded operator), for the self-adjoint Hamiltonian $H(s)$, which is bounded and differentiable for all $s \in [0,1]$. Then, the evolution of the initial state $\psi(0) \in Range P(0)$, according to Eq. (6), is such that in the adiabatic limit $\psi(s) \in Range P(s)$ for all s.

[1] We owe this argument to A. Ori.

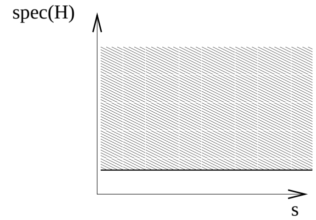

Figure 7: An Eigenvalue at Threshold

Remarks: The theorem is stated for bounded self adjoint operators $H(s)$. As it stands it does not apply to Schrödinger operator. The extension to unbounded operators is a technical problem which can be handled by known functional analytic methods. We choose not to phrase the result for the general case for several reasons. The first is that the technical issues will obscure the basic idea which is simple. The second is that the essence of the adiabatic theorem is an infrared problem. The unboundedness of Schrödinger operators is an ultraviolet problem. It is a conceptual advantage to keep the two issues separate.

The basic idea is to replace Kato's commutator equation, Eq. (15), by a definition of a new quantity $Y(s)$:

$$[H(s), X(s)] = [\dot{P}(s), P(s)] + Y(s), \tag{20}$$

and take $X(s)$ to be

$$X_\Delta(s) = \frac{1}{2\pi i} \int_\Gamma dz\, (1 - F_\Delta(s))\, R(z,s)\, \dot{P}(s) R(z,s)\, (1 - F_\Delta(s)). \tag{21}$$

where $F_\Delta(s)$ is an approximate characteristic function of $H(s)$, which is Δ localized near the relevant eigenvalue, whose range is in $Range\, P_\perp(s)$. $X_\Delta(s)$ is bounded, by construction, for $\Delta > 0$ and its norm diverges as $\Delta \to 0$. At the same time, and this is the crucial point, $\|Y_\Delta(s)\| \to 0$ provided $P(s)$ is finite dimensional. Chasing the argument of Kato one then finds that the adiabatic theorem holds, and the price one has to pay for the absence of a gap is the loss of control on the rate at which the adiabatic limit is approached. Instead of Eq. (8) on gets

$$\|\psi(s) - \phi(s)\| = o\,(1)\,. \tag{22}$$

That is, the error can be made arbitrarily small with τ, but the rate is undetermined.

We conclude with an interpretation of the result. For an isolated eigenvalue the gap in the spectrum protects against tunneling out of the spectral subspace. In the case that the eigenvalue in question is embedded in essential spectrum there is no gap to protect against tunneling out. But, since the essential spectrum is

associated with eigenfunctions supported near infinity, there is small overlap with the eigenfunction in question, and the protection against tunneling comes from this fact.

6 What Has Been Left Out

Adiabatic theorems of classical and quantum mechanics are a developed subject with rich and fertile history. In this short overview, based an a talk by one of us, we reviewed a small corner of this field, the one close to its foundations and characterized by elementary results. There are many beautiful and sophisticated results that we did not have the opportunity to review. These include: Classical adiabatic invariants for integrable systems to all orders [1, 18, 19]; Adiabatic invariants for chaotic systems [22, 7, 14]; Quantum adiabatic theorems to all orders [6, 17, 21, 15]; Landau-Zener formulas [13, 15]; Adiabatic invariants in scattering theory[20]; Adiabatic invariants in C^* algebras and models of quantum fields [9] and geometry and adiabatic curvature [5, 11].

Acknowledgments

This work was partially supported by a grant from the Israel Academy of Sciences, the Deutsche Forschungsgemeinschaft, and by the Fund for Promotion of Research at the Technion.

References

[1] V. Arnold, *Mathematical Methods of Classical Mechanics*, Springer (1980).

[2] J. E. Avron and A. Elgart, preprint, http://xxx.lanl.gov/abs/math-ph/9805022

[3] J. E. Avron, J. S. Howland and B. Simon, *Adiabatic theorems for dense point spectra*, *Comm. Math. Phys.* **128** (1990), 497–507.

[4] J. E. Avron, R. Seiler and L. G. Yaffe, *Adiabatic theorems and applications to the quantum Hall effect*, Comm. Math. Phys. **110** (1987), 33–49, (Erratum: Comm. Math. Phys. **153** (1993), 649-650).

[5] M.V. Berry, Proc. Roy. Soc. Lond. A **392**, 45, (1984); The quantum phase: Five years after, in *Geometric phases in physics* (A. Shapere and F. Wilczek, Eds., World Scientific, 1989).

[6] M.V. Berry, *Histories of adiabatic transition*, Proc. Roy. Soc. Lond. A **429**, 61-72, (1990).

[7] M.V. Berry and J.M. Robbins, *Chaotic classical and half classical adiabatic reactions: Geometric magnetism and deterministic friction*, Proc. Roy. Soc. Lond. A **442**, 659-672, (1993). Proc. Roy. Soc. A **392**, 45 (1984).

[8] M. Born and V. Fock, *Beweis des Adiabatensatzes*, Z. Phys. **51** (1928), 165–169.

[9] E. B. Davies and H. Spohn, *Open quantum systems with time-dependent Hamiltonians and their linear response*, J. Stat. Phys. **19**, 511, (1978).

[10] P. Ehrenfest, *Adiabatische Invarianten u. Quantentheorie*, Ann. d. Phys. **51**, 327 (1916)

[11] S. Golin, A. Knauf and S. Marmi, *The Hannay angles: Geometry, Adiabaticity and an example*, comm. Math. Phys. **123**, 95-122, (1989).

[12] G. Hagedorn, *Adiabatic Expansions near Eigenvalue Crossings*, Ann.Phys. **196**, 278-295 ,(1989).

[13] V. Jakšić and J. Segert, *On the Landau Zener formula for two-level systems*, J. Math. Phys. **34**, 2807-2820, (1993).

[14] C. Jarzinski, *Multiple-time-scale approach to ergodic adiabatic systems: Another look*, Phys. Rev. Lett. **71**, 839, (1993).

[15] A. Joye and C.E. Pfister, *Exponential Estimates in Adiabatic Quantum Evolution*, Proceeding of the XII ICMP, Brisbane Australia (1997); *Quantum Adiabatic Evolution*, in *On Three Levels*, M. Fannes, C. Maes and A. Verbure Editors, Plenum, (1994).

[16] T. Kato, *On the adiabatic theorem of quantum mechanics*, Phys. Soc. Jap. **5** (1958), 435–439.

[17] M. Klein and R. Seiler, *Power law corrections to the Kubo formula vanish in quantum Hall systems*, Comm. Math. Phys. **128** (1990), 141.

[18] A. Lennard, *Adiabatic Invariance to All Orders*, Ann. Phys. **6**, (1959), 261-276.

[19] P. Lochak and C. Meunier, *Multiphase Averaging for Classical systems*, Springer, (1988).

[20] H. Narnhofer and W. Thirring, *Adiabatic theorem in quantum statistical mechanics*, Phys. Rev. A **26**, 3646, (1982).

[21] G. Nenciu, *Linear Adiabatic Theory: Exponential Estimates*, Comm. Math. Phys. **152**, 479-496, (1993)

[22] E. Ott, *Goodness of ergodic adiabatic invariants*, Phys. Rev. Lett. **42** (1979), 1628-1631.